U.S. Department of Energy's
Office of Science

Program Area Presentation

Applied Mathematical Sciences (AMS)

Advanced Scientific Computing Research
Strategic Planning workshop

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22 July 2003

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Contribution of AMS program to Overall ASCR Strategic Goal

- "Forefront computational capabilities" to "extend the frontiers of science" ***requires***
  - Well-posed mathematical models (e.g., PDEs)
  - Mathematical analysis of model behavior
  - Solvable discrete versions (grid generation and discretization)
  - Efficient algorithms for solving the discretized models
  - Predictability analysis and uncertainty quantification for model reduction and to determine levels of confidence in the results
  - Engineering design optimization, discrete optimization problems, constrained optimization problems
  - New areas (dynamical systems, multiresolution analysis, multiscale mathematics, scalable algorithms) dictated by need and opportunity

Contribution of AMS program to Overall ASCR Strategic Goal (cont'd)

For 50 years, the Applied Mathematical Sciences research program has contributed to extending the frontiers of science in these applications areas:

- Chemically reacting flows / Combustion
- Climate Dynamics
- Materials Science
- Fundamentals of turbulence
- Subsurface flow
- Particle accelerator design
- Fusion reactor design and analysis
- Astrophysics
- Defense applications
- Biology
- Medical applications
- Infrastructure (e.g., power grids, transportation)
- …

Planning horizon for the AMS Program

- As a base research program, AMS *must* maintain balance between short-term (1-3 year) and long-term (3-10+ year) horizons
  - Some investments should have short- to medium-term payoff (e.g., improved solvers, preconditioners, meshes, software tools, …)
  - Many should target future barriers to scientific progress (e.g., multiphysics, multiscale, ultrascalable algorithms, asymptotically optimal methods, model reduction techniques, applications of discrete methods, hybrid methods, …)
- Short-term planning is relatively straightforward, long-term planning is fraught with challenges
  - Workshops help, but are not a panacea.

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Areas of research the AMS program currently invests in

- PDEs
- CFD
- Meshing and evaluation
- Adaptive Mesh Refinement
- Solvers (linear, nonlinear, eigenvalue)
- Optimization (continuous and discrete, constrained)
- Dynamical Systems
- High Performance Computation
- Automated Reasoning
- Boundary Integral Methods’
- Interface tracking methods (e.g., FronTier, Level Set)
- Statistics
- Predictability Analysis / Uncertainty Quantification
- Fast methods (e.g., FFTs, Fast Multipole, multigrid)
- Scalable methods
- Software tools (e.g., PETSc, TAO, EBChombo, MPSalsa, LOCA, Trilinos, Hypre, SuperLU, FronTier, …)
- Nanoscience
- Future star development
  - Five named fellowships at National Laboratories
  - Early Career Principal Investigator (ECPI) Program
  - Computational Sciences Graduate Fellowship (CSGF) Program

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How does the AMS program transfer knowledge or provide services to application scientists?

- AMS-supported researchers are…:
  - …actively collaborating with applications scientists, and/or…
  - …engaged in software development as both a testbed and deployment mechanism, and/or…
  - …also supported by funds such as SciDAC that are expressly for knowledge transfer, and/or…
  - …strongly motivated by a specific scientific or engineering challenge, and/or…
  - …have a strong connection to a DOE National Laboratory, or other scientific research facility
- The AMS program strives to balance immediate “relevance” with long-term research goals.

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AMS Program Strengths

- World-class research in applied mathematics for over 50 years
- Commitment from DOE/SC
- Dedication of scores of talented researchers in helping to nurture the program
- High visibility of AMS-supported researchers at (inter-)national meetings
- Strong research teams
- A DOE mission focus
- Interdisciplinary research motivation

AMS Program Weaknesses

- Insufficient speculative or risky investments
- Underinvestment or lack of investment in several critical areas:
    - Multiscale mathematics (impact in 5 years)
    - Ultrascalable algorithms (impact in 2 years)
    - Discrete mathematics (opportunities missed)
    - Statistics (impact immediate)
- Long-term stable program management
- Insufficient representation by women and minorities in the program
- In a recent review of Lab AMS programs, the most common criticism was that the programs were underfunded

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AMS Program Opportunities

- Recent (small) growth spurred by nanoscience initiative can be replicated
- Investments in multiscale mathematics now can remove roadblocks years down the road
  - Workshop series, co-chaired by Linda Petzold and Tom Hou, will begin in December
- Investments in discrete math/combinatorics could have huge payoffs for some applications (e.g., metabolic networks, homeland defense, infrastructure)
- Encouragement of more women and minorities in applied mathematics research could pay long-term dividends

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AMS Program Threats

- Erosion of ability to maintain identity from other agencies' research programs
- Increasing focus on value oriented management is inimical to fundamental research programs
  - What is the "net present value" of AMS?
  - Careless metrics have serious side-effects
    - Novel algorithms almost always lower both the time to solution and the (crude) parallel efficiency
  - Still, effectiveness of research programs must be measured
- Pressure to shorten the "payoff" horizon
- Pressure to skew balance of investments away from national laboratories and toward universities
- The 90/10 funding paradox at laboratories

AMS Program Gap Analysis

- Current gaps in the program include:
  - Multiscale mathematics
  - Ultrascalable algorithms
  - Discrete mathematics, and its role in mainstream scientific simulation
  - Statistics
  - Multiphysics
  - Insufficient representation of women and minorities in the research program